

Structure attributes must be viewed using STN Express query preparation.

s l11  
**REGISTRY INITIATED**  
 Instance data SEARCH and crossover from CAS REGISTRY in progress...  
 DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FILE SEARCH INITIATED 18:16:30 FILE 'REGISTRY'  
 FILE SCREEN SEARCH COMPLETED - 29 TO ITERATE

100% PROCESSED 29 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 REJECTED ITERATIONS: 257 TO 903  
 REJECTED ANSWERS: 0 TO 0

0 SEA SSS SAM L11

0 L12

s l11 full  
**REGISTRY INITIATED**  
 Instance data SEARCH and crossover from CAS REGISTRY in progress...  
 DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FILE SEARCH INITIATED 18:16:39 FILE 'REGISTRY'  
 FILE SCREEN SEARCH COMPLETED - 610 TO ITERATE

100% PROCESSED 610 ITERATIONS 1 ANSWERS  
 SEARCH TIME: 00.00.01

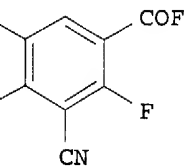
1 SEA SSS FUL L11

1 L14

display abs hitstr

CCÉSSION NUMBER: 1998:709043 CAPLUS  
DOCUMENT NUMBER: 129:316044  
TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and  
intermediates for its production  
INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter  
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
SOURCE: PCT Int. Appl., 30 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19717231	A1	19981029	DE 1997-19717231	19970424
AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
PRIORITY APPLN. INFO.:			DE 1997-19717231	A 19970424
			WO 1998-EP2175	W 19980414
			US 1999-403263	A3 19991015
			US 2001-814132	A1 20010321



3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II, and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

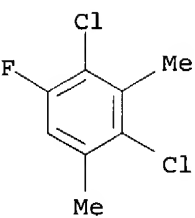
214774-61-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and chlorination of)

214774-61-5 CAPLUS

CN Benzene, 2,4-dichloro-1-fluoro-3,5-dimethyl- (9CI) (CA INDEX NAME)

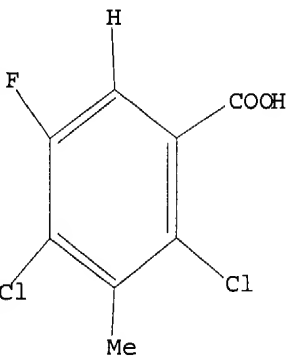


REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l1  
L1 HAS NO ANSWERS  
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1  
**REGISTRY INITIATED**  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 17:47:20 FILE 'REGISTRY'  
SCREENING  
SAMPLE SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.19

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 6 TO 266  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

L3 0 L2

=> s l1 full  
**REGISTRY INITIATED**  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 17:47:53 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 223 TO ITERATE

100.0% PROCESSED 223 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

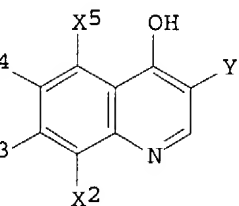
L4 1 SEA SSS FUL L1

5 2 L4  
> d 1-2 ibib abs hitstr

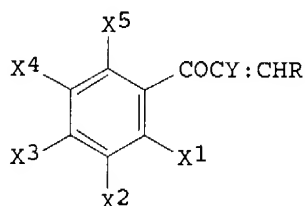
5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1988:94416 CAPLUS  
DOCUMENT NUMBER: 108:94416  
TITLE: Preparation of 4-hydroxyquinoline-3-carboxylates as  
intermediates for antibacterial 4-quinolone-3-  
carboxylates  
INVENTOR(S): Schriewer, Michael; Grohe, Klaus  
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.  
SOURCE: Ger. Offen., 11 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3615767	A1	19871112	DE 1986-3615767	19860510
EP 245690	A1	19871119	EP 1987-106123	19870428
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
US 4804760	A	19890214	US 1987-43663	19870428
JP 62273957	A2	19871128	JP 1987-110944	19870508
HU 44514	A2	19880328	HU 1987-2091	19870508
HU 197311	B	19890328		
US 4870182	A	19890926	US 1988-189559	19880503
PRIORITY APPLN. INFO.:			US 1985-795056	19851105
			DE 1986-3615767	19860510
			US 1987-43663	19870428

OTHER SOURCE(S): CASREACT 108:94416  
I



I



II

3 The title compds. I [Y = cyano, CO<sub>2</sub>R<sub>1</sub>, CONR<sub>2</sub>R<sub>3</sub>; R<sub>1</sub>, R<sub>2</sub> = H, alkyl; R<sub>3</sub> = R<sub>1</sub>, Ph; X<sub>2</sub>, X<sub>3</sub>, X<sub>4</sub>, X<sub>5</sub> = H, halo, NO<sub>2</sub>, cyano, alkyl, alkoxy, alkylthio, alkylsulfonyl, (un)substituted PhSO<sub>2</sub>] were prepared by cyclization of benzoylacrylate II (R = NHW; X<sub>1</sub> = halo, NO<sub>2</sub>, alkoxy, alkylthio, alkylsulfonyl, arylsulfonyl; W = H, CH<sub>2</sub>CH<sub>2</sub>Z; Z = cyano, CO<sub>2</sub>R<sub>4</sub>, CONR<sub>5</sub>R<sub>6</sub>; R<sub>4</sub>, R<sub>5</sub> = R<sub>1</sub>; R<sub>6</sub> = R<sub>3</sub>) by base in an aprotic solvent. Et (2,4-dichloro-5-fluoro-3-nitrobenzoyl)acetate (preparation given) was heated at 150-160° 3 h with HC(OEt)<sub>3</sub> and Ac<sub>2</sub>O to give II (R = OEt, X<sub>1</sub> = X<sub>3</sub> = Cl, X<sub>2</sub> = NO<sub>2</sub>, X<sub>4</sub> = F, X<sub>5</sub> = H) which was stirred 2 h with NH<sub>3</sub> in EtOH to give the corresponding enamine II (R = NH<sub>2</sub>). The latter was stirred 24 h with KOtBu in dioxane to give I (Y = CO<sub>2</sub>Et, X<sub>2</sub> = NO<sub>2</sub>, X<sub>3</sub> = Cl, X<sub>4</sub> = F, X<sub>5</sub> = H).

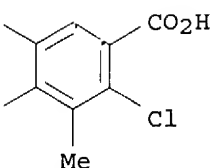
103877-68-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of antibacterial intermediates)

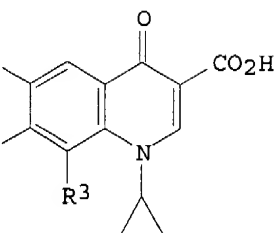
103877-68-5 CAPLUS

Benzoic acid, 2,4-dichloro-5-fluoro-3-methyl- (9CI) (CA INDEX NAME)

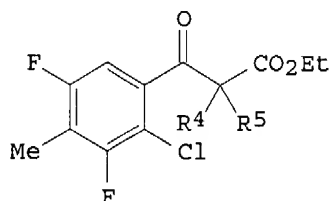


ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
 CESSION NUMBER: 1986:497345 CAPLUS  
 CUMENT NUMBER: 105:97345  
 TLE: 1-Cyclopropyl-1,4-dihydro-4-oxo-3-quinolinecarboxylic  
 acids  
 VENTOR(S): Grohe, Klaus; Schriewer, Michael; Zeiler, Hans  
 Joachim; Metzger, Karl Georg  
 TENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.  
 URCE: Ger. Offen., 41 pp.  
 CODEN: GWXXBX  
 CUMENT TYPE: Patent  
 NGUAGE: German  
 MILY ACC. NUM. COUNT: 2  
 TENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3441788	A1	19860515	DE 1984-3441788	19841115
AU 8549177	A1	19860522	AU 1985-49177	19851029
AU 572702	B2	19880512		
EP 181588	A2	19860521	EP 1985-114019	19851105
EP 181588	A3	19890201		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
US 4762844	A	19880809	US 1985-795056	19851105
CS 252835	B2	19871015	CS 1985-8132	19851112
FI 8504466	A	19860516	FI 1985-4466	19851113
ES 548843	A1	19861116	ES 1985-548843	19851113
CA 1260478	A1	19890926	CA 1985-495208	19851113
JP 61122272	A2	19860610	JP 1985-253881	19851114
ZA 8508733	A	19860730	ZA 1985-8733	19851114
BR 8505734	A	19860812	BR 1985-5734	19851114
HU 40422	A2	19861228	HU 1985-4347	19851114
HU 194178	B	19880128		
PL 145639	B1	19881031	PL 1985-256260	19851114
ORITY APPLN. INFO.:			DE 1984-3441788	19841115
HER SOURCE(S):		CASREACT 105:97345		



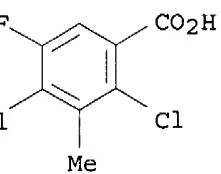
I



II

The title compds. (I; R1-R3 = H, NO2, alkyl, halo) were prepared as medical bactericides. Thus, 2,3,5,4-ClF2MeC6H5COC1 was condensed with (EtO2C)2CH2 to give benzoylmalonate II (R4 = H, R5 = CO2Et), which was sequentially hydrolyzed, decarboxylated, ethoxymethylenated with (EtO)3CH, and condensed with cyclopropylamine to give II [R4R5 = (cyclopropylamino)methylene]. The latter compound was cyclized and deesterified to give I (R1 = R3 = F, R2 = Me) (III). III had a min. inhibitory concentration of 0.06% against Staphylococcus aureus 133.  
 103877-68-5P

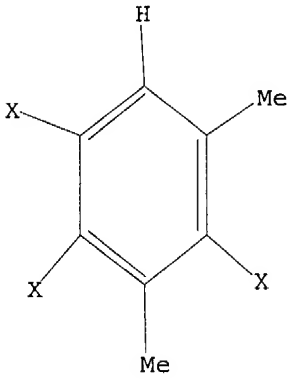
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and conversion of, to acid chloride)  
103877-68-5 CAPLUS  
Benzoic acid, 2,4-dichloro-5-fluoro-3-methyl- (9CI) (CA INDEX NAME)



=>  
Uploading C:\STNEXP4\QUERIES\7310.str

L1        STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1        STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1  
  **REGISTRY INITIATED**  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 13:34:49 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED -    5283 TO ITERATE  
  
  18.9% PROCESSED        1000 ITERATIONS                            0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    **\*\*COMPLETE\*\***  
                             BATCH    **\*\*COMPLETE\*\***  
PROJECTED ITERATIONS:        101303 TO    110017  
PROJECTED ANSWERS:                0 TO        0

L2                0 SEA SSS SAM L1

L3                0 L2

=> s l1 full  
  **REGISTRY INITIATED**  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 13:34:55 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 107048 TO ITERATE



L4 2 SEA SSS FUL L1

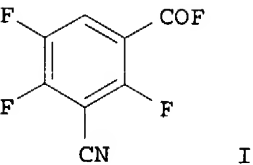
L5 2 L4

=> d 1-2 ibib abs hitstr

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1998:709043 CAPLUS  
DOCUMENT NUMBER: 129:316044  
TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and intermediates for its production  
INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter  
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
SOURCE: PCT Int. Appl., 30 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19717231	A1	19981029	DE 1997-19717231	19970424
AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
PRIORITY APPLN. INFO.:			DE 1997-19717231	A 19970424
			WO 1998-EP2175	W 19980414
			US 1999-403263	A3 19991015
			US 2001-814132	A1 20010321

GI

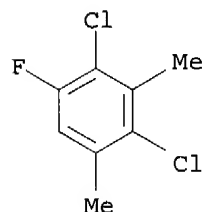


AB 3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from

5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II, and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

IT 214774-61-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and chlorination of)

RN 214774-61-5 CAPLUS  
 CN Benzene, 2,4-dichloro-1-fluoro-3,5-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

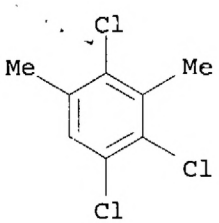
L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1978:597146 CAPLUS  
 DOCUMENT NUMBER: 89:197146  
 TITLE: Ring-chlorinated xylenes  
 INVENTOR(S): Blumenfeld, Georg; Riegger, Paul  
 PATENT ASSIGNEE(S): Dynamit Nobel A.-G., Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 18 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2702829	A1	19780727	DE 1977-2702829	19770125
US 4166075	A	19790828	US 1978-870400	19780118
JP 53092718	A2	19780815	JP 1978-6084	19780123
BE 863248	A1	19780516	BE 1978-184580	19780124
NL 7800863	A	19780727	NL 1978-863	19780124
FR 2377988	A1	19780818	FR 1978-1865	19780124
GB 1578411	A	19801105	GB 1978-2893	19780124
PRIORITY APPLN. INFO.:			DE 1977-2702829	19770125

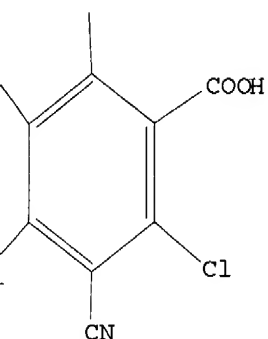
AB Xylenes were ring-chlorinated with Cl<sub>2</sub> in the presence of catalyst system of an iron halide or antimony halide with an aliphatic hydrocarbon, optionally halogenated, with an oxygen function, as cocatalyst. Thus, chlorinating p-xylene in CCl<sub>4</sub> containing FeCl<sub>3</sub> and cocatalyst MeOH, EtOH, PrOH, Me<sub>2</sub>CHOH, Me<sub>2</sub>CHCH<sub>2</sub>OH, Me<sub>3</sub>COH, trichloro-tert-Bu alc., HCO<sub>2</sub>H, AcOH, EtCO<sub>2</sub>H, Me<sub>2</sub>CHCO<sub>2</sub>H, or Me<sub>3</sub>CCO<sub>2</sub>H gave 0.1 and 0.6% 1,4-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>Cl (with AcOH and HCO<sub>2</sub>H), 54.0-78% 1,4-Me<sub>2</sub>C<sub>6</sub>H<sub>2</sub>Cl<sub>2</sub>-2,5, 8.1-22.6% 1,4-Me<sub>2</sub>C<sub>6</sub>H<sub>2</sub>Cl<sub>2</sub>-2,3, and 3.45-27.1% 1,4-Me<sub>2</sub>C<sub>6</sub>HCl<sub>3</sub>, with 88.2-99.1% conversion. Omitting a cocatalyst gave 4.8% 1,4-Me<sub>2</sub>C<sub>6</sub>H<sub>3</sub>Cl, 49.9% 1,4-Me<sub>2</sub>C<sub>6</sub>H<sub>2</sub>Cl<sub>2</sub>-2,5, 20.4% 1,4-Me<sub>2</sub>C<sub>6</sub>H<sub>2</sub>Cl<sub>2</sub>-2,3, and 22.9% 1,4-Me<sub>2</sub>C<sub>6</sub>HCl<sub>3</sub>, with 98% conversion.

IT 68266-71-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (improved chlorination procedure for)

RN 68266-71-7 CAPLUS  
 CN Benzene, 1,2,4-trichloro-3,5-dimethyl- (9CI) (CA INDEX NAME)



5 HAS NO ANSWERS  
5 STR



structure attributes must be viewed using STN Express query preparation.

s 16

**REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 17:51:17 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

0.0% PROCESSED 9 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

ALL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 9 TO 360  
PROJECTED ANSWERS: 0 TO 0

0 SEA SSS SAM L6

0 L7

s 16 full

**REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

ALL SEARCH INITIATED 17:51:37 FILE 'REGISTRY'  
ALL SCREEN SEARCH COMPLETED - 154 TO ITERATE

0.0% PROCESSED 154 ITERATIONS 1 ANSWERS  
ARCH TIME: 00.00.01

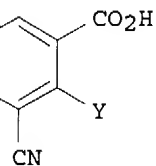
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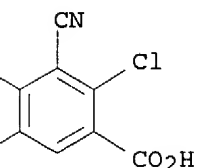
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ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
 SSION NUMBER: 1999:101296 CAPLUS  
 MENT NUMBER: 130:139168  
 E: Preparation of 3-cyano-2,4-dihalo-5-fluorobenzoic acid  
 by hydrolysis of the corresponding amides, nitriles,  
 or esters.  
 NTOR(S): Hallenbach, Werner; Marhold, Albrecht  
 NT ASSIGNEE(S): Bayer A.-G., Germany  
 CE: Ger. Offen., 18 pp.  
 CODEN: GWXXBX  
 MENT TYPE: Patent  
 UAGE: German  
 LY ACC. NUM. COUNT: 1  
 NT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19733243	A1	19990204	DE 1997-19733243	19970801
WO 9906360	A1	19990211	WO 1998-EP4468	19980718
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9891544	A1	19990222	AU 1998-91544	19980718
AU 744367	B2	20020221		
EP 1001929	A1	20000524	EP 1998-943740	19980718
EP 1001929	B1	20030326		
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BR 9811579	A	20000822	BR 1998-11579	19980718
JP 2001512098	T2	20010821	JP 2000-505122	19980718
NZ 502587	A	20020531	NZ 1998-502587	19980718
AT 235461	E	20030415	AT 1998-943740	19980718
PT 1001929	T	20030731	PT 1998-943740	19980718
ES 2190602	T3	20030801	ES 1998-943740	19980718
CN 1125042	B	20031022	CN 1998-807849	19980718
RU 2214998	C2	20031027	RU 2000-105245	19980718
US 6462218	B1	20021008	US 2000-463272	20000124
MX 200000861	A	20001109	MX 2000-861	20000125
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R SOURCE(S):		CASREACT 130:139168		

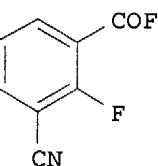


Title compds. (I; X, Y = halo) were prepared by hydrolysis of the  
 corresponding 3-cyano-2,4-dihalo-5-fluorobenzamides, 1,3-dicyano-2,4-  
 dihalo-5-fluorobenzenes, or 3-cyano-2,4-dihalo-5-fluorobenzoate esters.  
 Thus, 3-cyano-2,4-dichloro-5-fluorobenzamide was refluxed 3 h with concentrate  
 aqueous HCl to give 3-cyano-2,4-dichloro-5-fluorobenzoic acid.  
**117528-58-2P**  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (preparation of 3-cyano-2,4-dihalo-5-fluorobenzoic acid by hydrolysis of the  
 corresponding amides, nitriles, or esters)  
**117528-58-2 CAPLUS**



ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
 ESSION NUMBER: 1998:709043 CAPLUS  
 UMENT NUMBER: 129:316044  
 LE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and  
 intermediates for its production  
 ENTOR(S): Marhold, Albrecht; Wolfrum, Peter  
 ENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
 RCE: PCT Int. Appl., 30 pp.  
 CODEN: PIXXD2  
 UMENT TYPE: Patent  
 GUAGE: German  
 ILY ACC. NUM. COUNT: 1  
 ENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
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AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
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JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
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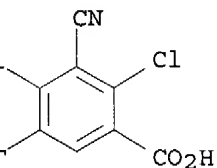
3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II, and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

117528-58-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

117528-58-2 CAPLUS

Benzoic acid, 2,4-dichloro-3-cyano-5-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:630824 CAPLUS

DOCUMENT NUMBER: 109:230824

TITLE: 8-Cyano-1-cyclopropylquinolonecarboxylic acids as antibacterial agents

INVENTOR(S): Schriewer, Michael; Grohe, Klaus; Petersen, Uwe; Haller, Ingo; Metzger, Karl Georg; Endermann, Rainer; Zeiler, Hans Joachim

PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 20 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

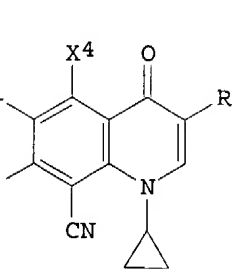
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

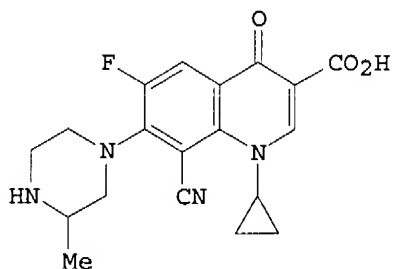
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DE 3702393	A1	19880811	DE 1987-3702393	19870128
US 4908366	A	19900313	US 1988-144884	19880114
EP 276700	A1	19880803	EP 1988-100503	19880115
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, SE				
CA 1314544	A1	19930316	CA 1988-557311	19880126
JP 63201170	A2	19880819	JP 1988-14771	19880127
US 5051418	A	19910924	US 1989-434666	19891113
US 5190955	A	19930302	US 1991-645751	19910125
PRIORITY APPLN. INFO.:			DE 1987-3702393	19870128
			US 1988-144884	19880114
			US 1989-434666	19891113

OTHER SOURCE(S): CASREACT 109:230824; MARPAT 109:230824



I



III

AB The title compds. [I; R = CO<sub>2</sub>H, cyano, CO<sub>2</sub>R<sub>1</sub>, CONR<sub>2</sub>R<sub>3</sub>; R<sub>1</sub> = alkyl; R<sub>2</sub> = H, alkyl; R<sub>3</sub> = R<sub>2</sub>, (un)substituted Ph; X<sub>1</sub> = H, NO<sub>2</sub>, alkyl, halo; X<sub>2</sub> = heterocyclyl; X<sub>4</sub> = H, halo, alkyl] were prepared as antibacterial agents (no data). 2,4,5,3-Cl<sub>2</sub>F(NC)C<sub>6</sub>HCOCH<sub>2</sub>CO<sub>2</sub>Et (preparation given) was heated 2 h at 150° with HC(OEt)<sub>3</sub> in Ac<sub>2</sub>O to give 2,4,5,3-Cl<sub>2</sub>F(NC)C<sub>6</sub>HCOC(:CHR<sub>4</sub>)CO<sub>2</sub>Et (II; R<sub>4</sub> = OEt) which was stirred 2 h with cyclopropylamine in EtOH to give II (R = cyclopropylamino). The latter was stirred 24 h in dioxane containing KOCMe<sub>3</sub> to give, after saponification, I (R = CO<sub>2</sub>H, X<sub>1</sub> = F, X<sub>2</sub> = Cl, X<sub>4</sub> = H) which was heated 3 h in dioxane with 2-methylpiperazine to give title compound III. Tablets were prepared each containing III 583.0, cellulose 55.0, starch 72.0, polyvinylpyrrolidone 30.0, silica 5.0, and Mg stearate 5.0 mg coated with poly(O-hydroxypropyl-O-methyl)cellulose 6.0, Macrogol 4000 2.0, TiO<sub>2</sub> 2.0 mg, and polyethyleneglycol (no amount given).

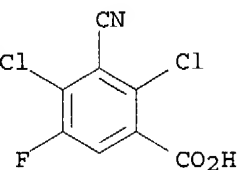
IT 117528-58-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

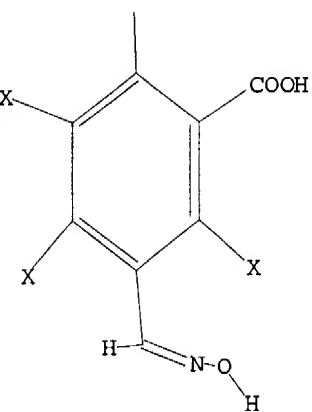
(preparation and reaction of, in preparation of antibacterial agents)

RN 117528-58-2 CAPLUS

CN Benzoic acid, 2,4-dichloro-3-cyano-5-fluoro- (9CI) (CA INDEX NAME)







Structure attributes must be viewed using STN Express query preparation.

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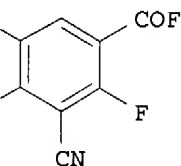
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13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1998:709043 CAPLUS  
DOCUMENT NUMBER: 129:316044  
TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and  
intermediates for its production  
INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter  
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany  
SOURCE: PCT Int. Appl., 30 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
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AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
R:	AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE			
JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
US 2001023300	A1	20010920	US 2001-814132	20010321
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US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
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			WO 1998-EP2175	W 19980414
			US 1999-403263	A3 19991015
			US 2001-814132	A1 20010321



3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II, and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

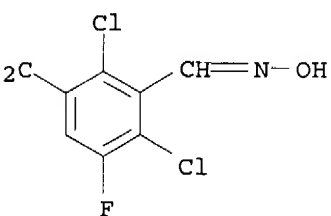
214774-57-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and chlorination-dehydration of)

214774-57-9 CAPLUS

Benzoic acid, 2,4-dichloro-5-fluoro-3-[(hydroxyimino)methyl]- (9CI) (CA  
INDEX NAME)



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT